**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

# STRUCTURE AND SYLLABUS OF MSc COURSEWORK

# TO BE DISCUSSED IN THE

# BOARD OF STUDIES (CENTRE FOR COMPUTATIONAL SCIENCES)

# FOR

# MSc Chemistry (Computational Chemistry)

**2017-19**

**Central University of Punjab**
**Bathinda-151001**

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

## Eligibility Criterion and number of available seats for M.Sc. Chemistry (Computational Chemistry) approved by BOS

Bachelor's degree in Science with Chemistry as a subject with 55% marks in aggregate from a recognized Indian or foreign university. The Centre offers 15 seats for Post-Graduation in Chemistry (Computational Chemistry)

# CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001
## Centre for Computational Sciences

### Programme Objective:

The objective of M. Sc. Chemistry (Computational Chemistry) Programme is that a student graduating after successful completion of the Programme shall be proficient in understanding the intricacies of relationship and interplay between Chemistry and Computational Sciences. This course is expected to enable the students to attain a Master's level understanding of Chemistry in general and Computational Chemistry in particular. In addition, based on the research training provided in this course, the students should be enabled to understand concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out further research in higher degrees. In addition, extensive stress on logic based discipline would ensure development of scientific temperament among the students. Therefore graduated students of MSc Chemistry (Computational Chemistry) would be valuable asset for the nation by virtue of their scientific abilities. The student can expect successful career/employment in academic / research / industry by undertaking this course. A special effort has been made to enable the student clear national level tests for teaching ability and research fellowships especially, CSIR-NET.

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## M. Sc. Chemistry (Computational Chemistry)

| Semester I | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| S. No. | Paper Code | Course Title | Course Type | L | T | P | Cr | % Weightage | | | | e |
| | | | | | | | | a | b | c | d | |
| | | Research Methodology | FC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| 1 | CSC.501 | Scientific Programming | CC | 3 | 2 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 2 | CSC.451 | Mathematics for Chemists | FC | 3 | 2 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 3 | CSC.452 | Chemical Biology | FC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| 4 | CSC.502 | Scientific Programming Lab | CC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| 5 | CHL.508 | Physical Chemistry-I | CC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| | | Organic Chemistry- Practical | CC | - | - | 4 | 2 | - | - | - | - | 50 |
| | | Inorganic Chemistry-Practical | CC | - | - | 4 | 2 | - | - | - | - | 50 |
| 6 | XXX | Interdisciplinary Elective | EC | 2 | - | - | 2 | 10 | 15 | 15 | 10 | 50 |
| Choose any one of these courses: | | | | | | | | | | | | |
| 7 | CHL.504 | Inorganic Chemistry-I | EC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| 8 | CHL.506 | Organic Chemistry-I | EC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| Interdisciplinary course offered for other centres: | | | | | | | | | | | | |
| 10 | CSC.503 | Chemistry without test tube | EC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| | | Total | | | | | 20 | | | | | 500 |

**Please Note: Subject codes with "CHL" prefix shall be conducted by the Centre for Chemical Sciences and the Centre for Computational Sciences shall conduct courses with "CSC" prefix.**

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| Semester II | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **S. No.** | **Paper Code** | **Course Title** | **Course Type** | **L** | **T** | **P** | **Cr** | **% Weightage** | | | | **e** |
| | | | | | | | | **a** | **b** | **c** | **d** | |
| | | Fundamentals of Molecular Simulations | CC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| | | Molecular Simulations Lab | CC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| 1 | LBI.524 | Perl Primers for Data Analysis | CC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| 2 | LBI.527 | Data Analysis with PERL | CC | - | - | 2 | 1 | - | - | - | - | 25 |
| 3 | CSC.504 | Quantum Chemistry — I | CC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 4 | CSC.505 | Statistical Mechanics — I | CC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 5 | CHL.524 | Physical Chemistry-II | CC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| | | Inorganic Chemistry-II | EC | 4 | 1 | 0 | 4 | 25 | 25 | 25 | 25 | 100 |
| | | Organic Chemistry-II | EC | 4 | 1 | | 4 | 25 | 25 | 25 | 25 | 100 |
| | | Seminar in Computational Sciences | FC | - | - | 4 | 2 | - | - | - | - | 50 |
| 6 | CHP.525 | Practical Physical Chemistry - II | CC | - | - | 4 | 2 | - | - | - | - | 50 |
| 7 | LBI.623 | Scientific Writing and IPR | CC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| 8 | XXX | Humanities for Science Students | EC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| **Choose any one of these courses:** | | | | | | | | | | | | |
| 9 | CHL.521 | Inorganic Chemistry — II | EC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| 10 | CHL.523 | Organic Chemistry — II | EC | 3 | - | - | 3 | 25 | 25 | 25 | 25 | 75 |
| | | Total | | | | | 24 | - | - | - | - | 600 |

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| Semester III | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **S. No.** | **Paper Code** | **Course Title** | **Course Type** | **L** | **T** | **P** | **Cr** | **Weightage** | | | | **e** |
| | | | | | | | | **a** | **b** | **c** | **d** | |
| 1 | CSC.453 | Computational Methods | FC | 3 | 2 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 2 | CSC.454 | Computational Methods Lab | FC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| 3 | CSC.601 | Electronic Structure Theory | CC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 4 | CSC.602 | Electronic Structure Theory Lab | CC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| 5 | CSC.603 | Fundamentals of Molecular Simulations | CC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 6 | CSC.604 | Molecular Simulations Lab | CC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| 7 | CSC.499 | Seminar in Computational Science | FC | - | - | 4 | 2 | - | - | - | - | 50 |
| | | Introduction to Scripting | FC | 2 | - | - | 2 | 25 | 25 | 25 | 25 | 50 |
| | | Scripting Lab | FC | - | - | 4 | 2 | - | - | - | - | 50 |
| | | Dissertation Research | CC | - | - | 12 | 6 | - | - | - | - | 150 |
| Choose any one of these courses | | | | | | | | | | | | |
| 8 | CSC.605 | Molecular Spectroscopy | EC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 9 | CSC.606 | Introduction to Biochemistry | EC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 10 | CSC.607 | Density Functional Theory | EC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 11 | CSC.608 | Introduction to Quantum Dynamics | EC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 12 | CSC.609 | Statistics for Chemical and Biochemical Applications | EC | 4 | 1 | - | 4 | 25 | 25 | 25 | 25 | 100 |
| | Total | | | | | | 24 | | | | | 600 |

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| Semester IV | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **S. No.** | **Paper Code** | **Course Title** | **Course Type** | **L** | **T** | **P** | **Cr** | **Weightage** | | | | **e** |
| | | | | | | | | **a** | **b** | **c** | **d** | |
| 1 | **CSC.611** | M.Sc. Project Work | CC | - | - | 24 | 12 | - | - | - | - | S/US |
| 2 | **CSC.612** | Biomolecular Modeling and Drug Designing Lab | CC | - | - | 4 | 2 | 25 | 25 | 25 | 25 | 50 |
| Select any two of the following courses: | | | | | | | | | | | | |
| 2 | **CSC.613** | Biomolecular Modeling and Drug Designing | EC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 4 | **CSC.614** | Advanced Statistical Mechanics and Molecular Reaction Dynamics | EC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 5 | **CSC.615** | Modeling Polymeric Materials | EC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| 6 | **CSC.616** | Physical Organic Chemistry | EC | 4 | - | - | 4 | 25 | 25 | 25 | 25 | 100 |
| | | | | | | | 22 | | | | | 250 |

**a: Continuous Assessment:**Subjective by enlarge
**b: Mid-Term Test-1:**Based on Objective Type & Subjective Type Test
**c: Mid-Term Test-2:**Based on Objective Type & Subjective Type Test
**d: End-Term Exam (Final):**Based on Objective Type Tests
**e:** Total Marks
**L:** Lectures **T:** Tutorial **P:** Practical **Cr:** Credits
**FC:** Foundation Course **CC:** Core Course **EC:** Elective course

**The subject in red font signifies that these subjects are proposed to be replaced with those in greeen font. The subjects in blue font are proposed to be shifted from second to the third semester.**

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## M.Sc. Chemistry (Computational Chemistry) Course Structure

### SEMESTER- I

**Objective and Expected Learning Outcomes:** The course structure of semester I of this Programme is designed to ensure complete overlap with courses taught to students of M. Sc. Chemical Sciences and M. Sc. Chemical Sciences (Medicinal Chemistry). Thus, the first semester includes courses in inorganic, organic, physical chemistry and some interdisciplinary courses and is designed to provide breadth of knowledge in the discipline of Chemistry. The breadth knowledge gained in this semester will help students better understand the interdisciplinary area of Computational Chemistry. The list of courses to be taught in this semester is provided below, and is adapted from the Course structure of M. Sc. Chemical Sciences programme currently running in the Centre for Computational Sciences of CUPB.

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**Course Title:** Scientific Programming
**Paper Code:** CSC.501
**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 2 | 0 | 4 | 100 |

**Course Objective and Learning Outcomes:** The objective of this course is to introduce students to the art of scientific programming. The theory part practical aspects of scientific programming languages Fortran and C will be taught to students in this course.

**Unit I** **(18)**

**Introduction to Computers and Fortran and C languages:** History and evolution of Fortran and C languages, Basic elements of Fortran and C: Character sets, structure of statements, Structure of a Fortran and C Program, compiling, linking and executing the Fortran and C programs.

**Unit II** **(18)**

Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

**Unit III** **(18)**

Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.

**Unit IV** **(18)**

Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran and C.

**Books Recommended:**

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997).
5. Foy, Mastering Perl First Edition, O'Reilly Media (2007).

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**Course Title: Mathematics for Chemists**
**Paper Code: CSC.451**
**Total Lectures: 72**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Course Objective and Learning Outcomes:** The objective of this course is to cover the basic mathematical techniques that are commonly used by chemist. After, completion of this course will help the students to solve the complex problems in group theory, quantum chemistry, statistical thermodynamics, molecular spectroscopy, and chemical kinetics etc in the advance stage of computational chemistry program.

**Unit I: Vectors, matrices and determinants (18)**

Vectors: Vectors, dot, cross and triple products etc. the gradient, divergence & curl, vector calculus.
Applications: Two body peoblem, center of mass and relative coordinates, Potentials.
Matrix algebra: addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew symmetric, hermitian, skew hermitian, unit, diagonal, unitary etc) and their properties, matrix equations: homogeneous, non homogeneous linear
equations and conditions for the solution, linear dependence and indepedence, introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants, introduction to tensors.
Applications: Slater determinants, Huckel Molecular Orbital Theory, Polarizability and Magnetic Susceptibility.

**Unit II: Differential calculus: (09)**

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties.
Applications: Maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell distribution.

**Unit III: Integral calculus: (09)**

basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations
Applications: Cartesian to spherical polar, curve sketching.

**Unit IV: Elementary differential equations: (18)**

variables-separable and exact first-order differential equations, homogeneous, exact and linear equations, solutions of differential equations by the power series method, Fourier series,
solutions of harmonic oscillator and legendre equation etc, spherical harmonics, second order differential equations and their solutions.
Applications: chemical kinetics, secular equilibria, quantum chemistry etc,

**Unit V: Permutation and probability: (18)**

permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, example from the kinetic theory of gases etc, curve fitting (including least squares fit etc) with a general polynomial fit.
Statistics: mean, median, mode, standard deviations, and Correlation coefficient, student t-test.

**Books Recommended:**


1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.
7. Mathematics for Chemists: Bhupendra Singh, Pragati Prakashan

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**Course Title: Chemical Biology**
**Paper Code: CHL.501**
**Total Lectures: 36**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 2 | 0 | 0 | 2 | 50 |

**Course Objective and Learning Outcomes:** To impart knowledge of molecular structure and interactions present in various bio-molecules that assist in functioning and organization of biological cell. After, completion of this course the students will acquire knowledge of molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids, the organization and working principles of various components present in living cell, and the physical principles of structure, function, and folding of biomolecules.

**Unit I** **(09)**

Introduction: Cell structure and functions, thermodynamics and kinetics of biological processes, ATP. water – physical properties and structure of water molecules, Interactions in aqueous solutions, Role of water in life, pH, Biological buffers, solution equilibria, Henderson - Hasselbalch equation, Hofmeister series, Chaotropic and kosmotropic ions/co-solvents.

**Unit II** **(09)**

Amino Acids and Peptides : Classification and properties of amino acids, peptide and polypeptides, primary structures, structure of peptide bond, synthesis of peptides, N-terminal,
C-terminal and sequence determination.
Carbohydrates: Biologically important monosaccharides, disaccharides and polysaccharides, glycoproteins , role of sugars in biological recognition.

**Unit III** **(09)**

Proteins: Secondary structure of proteins with emphasize on supramoelcular characteristics of
α-helix, β-sheets, supersecondary structure and triple helix structure of collagen, tertiary structure of protein-folding, quaternary structureof protein, protein misfolding and conformational diseases.
Catalysis and binding in enzymes, ligand - protein interactions, membranes, ribosomes and multienzyme complexes as supramolecular complexes.

**Unit IV:** **(09)**

Nucleic Acids: Purine and pyrimidine bases, nucleotides, nucleosides, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA, different types of RNA and their functions, the chemical basis for heredity, overview of replication of DNA, transcription, translation and genetic code, genome sequencing and PCR techniques.

Lipids: Lipid classification, lipid bilayers, liproproteins - composition. high density (HDL) and low-density (LDL) lipoproteins and function, membrane proteins - integral membrane proteins, lipid linked proteins, peripheral proteins, overview of membrane structure and assembly, liposomes, their biological functions.

**Books Recommended:**


1.Voet, D.J., Voet, J.G., Pratt, C.W., Principles of Biochemistry, 3rd edition, 2008, John Wiley,.
2. Berg, J.M., and Tymoczko, J.L., Stryer, L., Biochemistry, 6th edition, 2007, W.H. Freeman,.
3. Garrett, R.H., Grisham, C.M., Biochemistry, Brooks/Cole, 4th edition, 2014, Cengage Learning,.
4. Conn, E.E., and Stump, F., Outlines of Biochemistry, 5th edition, 2006, John Wiley.

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**Course Title:** Scientific Programming Lab
**Paper Code:** CSC.502
**Total Lectures:** 36

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| - | - | 4 | 2 | 50 |

**Course Objective and Learning Outcomes:** The objective of this course is to introduce students to the art of scientific programming. The practical aspects of scientific programming languages Fortran and C will be taught to students in this course.

**Unit I** **(09)**

**Introduction to Computers and Fortran and C languages:** History and evolution of Fortran and C languages, Basic elements of Fortran and C: Character sets, structure of statements, Structure of a Fortran and C Program, compiling, linking and executing the Fortran and C programs.

**Unit II** **(09)**

Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.

**Unit III** **(09)**

Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran and C.

**Unit IV** **(09)**

Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination.

**Numerical Computation:** Integration using the Simpson's method, the Gaussian quadrature method, Solution of first order differential equations using the Rung-Kutta method, Numerical first order differentiation of a given function.

**Books Recommended:**


1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997).
5. Foy, Mastering Perl First Edition, O'Reilly Media (2007).

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**Course Title: Physical Chemistry I**
**Paper Code: CHL.508**
**Total Lectures: 54**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**Course Objective and Learning Outcomes:** The objective of this course is that students learn the principles of physical chemistry, which is a fundamental branch of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in physical chemistry.

**Unit 1** **(10)**

**Thermodynamics:** Concepts involved in first, second and third law of thermodynamic, Helmholtz and Gibbs Energies, Maxwell relations, equilibrium constant, temperature-dependence of equilibrium constant, Van't Hoff equation.

**Unit 2** **(10)**

**Partial Molar Properties and Fugacity:** Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs- Duhem equation, real gases, fugacity, its importance and determination, standard state for gases.

**Solid-Liquid Solutions:** Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

**Unit 3** **(12)**

**Thermodynamics of Simple Mixtures:** Thermodynamic functions for mixing of perfect gases. chemical potential of liquids. raoult's law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities. Clausius-clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

**Unit 4** **(22)**

**Statistical Thermodynamics:** Thermodynamic probability and entropy, maxwell-boltzmann, bose-einstein and fermi-dirac statistics. partition function, molar partition function, thermodynamic properties in term of molecular partition function for diatomic molecules, monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function. monoatomic solids, theories of specific heat for solids.

**Books Recommended**


Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 5th/3rd Edition, 2011, Macmillan.
Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books.
Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4th Edition, 2004, Wiley-Interscience Publication.
Engel, T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
Puri, B.R., Sharma L.R. and Pathania, M.S. Principles of Physical Chemistry, 46th Edition, 2013, Vishal Publishing Company.
Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics 6th edition, 2013, Vikas Publishing
Rajaram, J. and Kuriacose, J. C. Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, 2013, Pearson Education.
Laurendeau N. M. Statistical Thermodynamics: Fundamentals and Applications, 2005, Cambridge University Press.
Nash, L. K. Elements of Statistical Thermodynamics, 2nd Edition, 2012, Dover Publication Inc.
Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.


**Course Title: Inorganic Chemistry I**
**Paper Code: CHL.504**
**Total Lectures: 54**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

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**Course Objective and Learning Outcomes:** The objective of this course is that students learn the principles of inorganic chemistry, which is a fundamental branch of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

**Unit I** **(10)**

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constant and their interaction, trends in stepwise constants,factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by spectrophotometry and potentiometric (pH) methods.

**Unit 2** **(15)**

Reaction Mechanisms of Transition Metal Complexes

Introduction,potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere, Berry pseudorotation.

**Unit 3** **(15)**

Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties of transition metal ions and free ions presentive, effects of L-S coupling on magnetic properties, temperature independent paramagnetism(TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), quenching of orbital angular momentum by crystal fields in complexes in terms of termsplitting. effect of spin-orbit coupling and A, E & T states mixing.

**Unit 4** **(14)**

Crystal Fields Splitting

Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of pn, dn ions, determination of the ground state terms for pn, dn, fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters (λ) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, variation of the Racah parameter, spectrochemical series, band intensities, factors influencing band widths.

**Books Recommended:**


1. Cotton, F.A. and Wilkinson G. Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4thedition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2ndedition, 2005 (reprinted),Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2ndedition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J.Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, SpringerverlagNew York Inc., 1977.
6. Miessler,G. L.andTarr, D. A. Inorganic Chemistry,4thedition, 2011, Pearson Education.
7. Figgis,B.N. Introduction to Ligand Field, 1966Wiley Eastern.
8. Drago,R.S. Physical Method in Chemistry, 1965, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5thedition, 2010, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
11. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2ndedition, 1993, Affiliated East West Press.
12. Drago, R. S. Physical Methods for Chemists, 2ndedition, 1992, Saunders College Publishing.


**Course Title: Organic Chemistry I**

**Paper Code: CHL.506**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Total Lectures: 54**

**Course Objective and Learning Outcomes:** The objective of this course is that students learn the principles of organic chemistry, which is a fundamental branch of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in organic chemistry.

**Unit 1** **(16)**

Stereochemistry: Elements of symmetry, chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, configurational notations of simple molecules, D/L, R/S, E/Z and cis/trans configurational notations, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity, conformation of sugars.

**Unit 2** **(14)**

Aliphatic nucleophilic substitution reaction: The SN2, SN1, mixed SN2 and SN1 and SET mechanism, the SNi mechanism. nucleophilic substitution at an allylic, aliphatic and vinylic carbon. reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between SN2 and SN1 mechanisms, Vilsmeier–Haack reaction.

Aromatic nucleophilic substitution: The SNAr, bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling.

**Unit 3** **(12)**

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

**Unit 4** **(12)**

Addition to carbon-hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, Arndt-Eistert synthesis, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard reagent, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

**Books Recommended:**


1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2nd edition, 2012, Oxford University Press.
2. Finar, I.L. Organic Chemistry Volume 1, 6th edition, 2012, Pearson Education UK.
3. McMurry J. Organic Chemistry, 8th edition, 2011 Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edition, 2013, John Wiley & Sons.
5. Ahluwalia, V. K. and Parashar R. K. Organic Reaction Mechanism, 4th edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
6. Bansal, R. K. A text book of Organic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
7. Bansal R.K. Organic Reaction Mechanism, 2010, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3rd edition, 2010, New Age International, New Delhi.
9. Kalsi, P.S. Stereochemistry: Conformation and Mechanism, 2010, New Age International Ltd, New Delhi.

10. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3rd edition, 1998, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6th edition, 2011, Prentice- Hall of India, New Delhi.
12. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3rd edition, 2009, Macmillan India Ltd., New Delhi.
13. Robert, J. D. and Casereo, M.C. Basic principle of Organic Chemistry, 2nd edition, 1977, Addison-Wesley.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A.Organic Chemistry. 11th edition, 2013, John Wiley and Sons, Inc.
15. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6th edition, 1997, Prentice Hall.
16. Eliel, E. L. and Wilen, S. H. Stereochemistry of Organic Compounds, 1994, John Wiley & Sons.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Chemistry without Test Tube (ID)
**Paper Code:** CSC.503
**Total Hours:** 36

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 36 | 0 | 0 | 2 | 50 |

**Course objective:** The aim of this course is to present a qualitative theory of chemical bonding stressing the physical processes which occur on bond formation. Although this is a course in chemistry full of mathematics but, we will use little mathematics to understand the chemical physics behind bonding and reactions.

**Unit-I** **(09)**

**How Science Deals with Complex problems:** Level in science, what are molecules made of, interaction between atoms, simplest examples: H2 and LiH. Thinking in 3D, must we use quantum theory.

**Unit-II** **(09)**

**Electronic Structure:** What we know about atoms and molecules; atomic electronic structure, empirical chemistry; what is an orbital (atomic and molecular). Strategy for electronic structure, the Pauli principle and orbitals. Polyatomic Molecules:Methane, electronic structre of methane, shape of the methane molecule, chemist's description of methane.

**Unit-III** **(09)**

**Lone pairs of electrons:** Why are Not all electrons involved in bonding? What is a lone pair? Shapes of the simple molecules.

**Organic molecules with multiple bonds:** Double and triple bonds, ethene and methanal, reactivity of a double bond.

**Diatomics with multiple bonds:** N2, CO, O2

**Dative Bonds:** Solvation, reactive lone paire

Delocalized electronic substructures: The benzene molecule, delocalized electrons.

**Unit-IV** **(09)**

**Reactions:** What makes a reaction to go? Formation of H2 from H+ and H-.Formation of lithium borohydride. Nucleophilic, elimination and addition reactions.

**Recommended Books:**


1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
2. A. R. Leach, Molecular Modelling Principles and Applications, Prentice Hall (2001).
3. Introduction to Computational Chemistry, F. Jensen, 2nd edition, Wiley-Blackwell (2006).
4. Quantum Chemistry: A Unified Approach, D. B. Cook, 2nd edition, Imperial College Press (2012).
5. Why Chemical Reactions Happen, J. Keeler, P. Wothers, Oxford University Press (2003).
6. Reaction Dynamics, M. Brouard, Oxford Chemistry Primers (1998).

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

## SEMESTER II

**Objective and Expected Learning Outcomes:** The course structure of semester II of this Programme is designed to ensure some overlap with courses taught to students of M. Sc. Chemical Sciences and M. Sc. Chemical Sciences (Medicinal Chemistry). This semester includes advanced courses in inorganic, organic, physical chemistry and some interdisciplinary courses and is designed to provide breadth of knowledge in the discipline of Chemistry. In addition, the breadth knowledge gained in this semester will help students better understand the interdisciplinary area of Computational Chemistry. The list of courses to be taught in this semester is provided below, some of which are adapted from the Course structure of M. Sc. Chemical Sciences programme currently running in the Centre for Chemical Sciences of CUPB.

**Course Title: Perl Primers for Data Analysis**
**Paper Code: LBI.524**
**Total Lecture:** 54

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**Course Objective and Learning Outcomes:** The objective of this subject is to ensure that student learns basic Unix and PERL programming.

**Unit: 1** **(14)**

Scripting languages and introduction: Getting comfortable with the UNIX shell, Basic shell commands, Unix shell scripting programming languages, Origin of PERL as a scripting language, Installation on various OS, Integrated Development Environment, The Comprehensive PERL Archive Network, BioPerl, Getting started in PERL coding, Running PERL programs.

**Unit: 2** **(14)**

PERL Basics: Scalar variables, Syntax and semantics, Processing scalar variables, Iteration with while construct,Variable containers, Loops, Conditional statements, Introducing Patterns, Reading and writing files, Case study: Making Motif Search tool.

**Unit: 3** **(14)**

Advance data structure and programming in PERL: Arrays, Hashes, Sub-routines, Getting organized: Visibility and Scope of big programs, Modules, Case study: Parsing NCBI GenBank records.

**Unit: 4** **(10)**

Regular expression and Text mining: The Match Operator, Match Operator Modifiers, The Substitution Operator, Substitution Operator Modifiers, Translation, Translation Operator Modifiers, More complex regular expressions, Case study: UniProt database parsing.

**Books Recommended:**

1. Moorhouse M, Barry P (2005): Bioinformatics Biocomputing and Perl: An Introduction to Bioinformatics Computing Skills and Practice, Book, John Wiley & Sons
2. Dwyer R. A. (2003): Genomic Perl: From Bioinformatics Basics to Working Code, Volume 1, Book, Cambridge University Press
3. Tisdall J (2003): Mastering Perl for Bioinformatics, Book, O'Reilly
4. Hietaniemi J, John Macdonald J, Orwant J (1999): Mastering Algorithms with Perl, Book, O'Reilly
5. Bradnam K & Korf I (2012): Unix and Perl Primer for Biologists, Web tutorial at http://korflab.ucdavis.edu/Unix_and_Perl/current.html
6. Robert's PERL tutorial http://www.physics.rutgers.edu/~kotliar/perltut.html
7. Collection of PERL tutorials at http://perl-tutorial.org/

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Data Analysis with PERL**
**Paper Code: LBI.527**
**Total Lecture:** 36

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

**Course Objective and Learning Outcome:** The objective of this subject is to ensure that students able to write their own programs in PERL for data mining and analysis.

1. Unix Shell scripting, Grep, AWK and SED

2. Printing various number sequences

3. Reading and writing files

4. Searching patterns in files

5. Programming Motif Search tool

6. Sorting algorithm

7. Counting GC and amino acid contents in sequence files

8. Translating gene sequence into protein using Hashes

9. Creating and using modules

10. Parsing BLAST result files

11. Parsing NCBI GenBank records

12. UniProt records to annotation tables

**Books Recommended:**

1. Moorhouse M, Barry P (2005): Bioinformatics Biocomputing and Perl: An Introduction to Bioinformatics Computing Skills and Practice, Book, John Wiley & Sons
2. Hietaniemi J, John Macdonald J, Orwant J (1999): Mastering Algorithms with Perl, Book, O'Reilly

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Quantum Chemistry-I
**Paper Code:** CSC.504
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Objective and Learning Outcomes:** This is a fundamental course for students who specialize in Computational Chemistry. The objective of this course is that students learn the basic concepts of quantum chemistry and apply them to study simple problems that have analytical solutions. In addition, the course will introduce the students towards basic ideas on solving problems in molecular quantum mechanics, which will, in turn, prepare them to take the next advanced level course of Computational Chemistry.

**Unit I** **(20)**

**Fundamental Background:** Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor. Angular momentum, eigenvalues of angular momentum operator, Particle in a Ring, Hydrogen Atom.

**Unit II** **(14)**

**Approximate Methods:** Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

**Unit III** **(18)**

**Symmetry Point Groups:** Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction of character tables for c2v and c3v groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

**Unit IV** **(20)**

**Atomic and Molecular Structure:** many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Born-Oppenheimer approximation. Molecular orbital treatment for H2+.MO treatment of homo- and hetero nuclear diatomic molecules.Hückel mo treatment of simple and conjugated polyenes and alternate hydrocarbons.

**Books Recommended:**


1. Quantum Chemistry, I.N. Levine, 5th edition, Pearson Educ., Inc. New Delhi (2000).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
3. Valence Theory, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd edition, John Wiley (1965).
4. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
5. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons (2008).
6. Molecular Symmetry and Group Theory, R. L. Carter, J. Wiley (1998).
7. Group Theory and Chemistry, D. M. Bishop, Dover Publications (1993).
8. Quantum Chemistry, J. P. Lowe, and Peterson, K., Academic Press (2005).

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Statistical Mechanics I**
**Paper Code:** CSC.505
**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Unit I: (18)**

**Mathematical Review of Classical Mechanics:**
Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations
Classical approach to Ensembles:
Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and it's ensembles
Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

**Unit II: (18)**

**Elementary Probability Theory**
Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem
Distributions & Fluctuations:
Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable

**Unit III: (18)**

**Basic Thermodynamics:** Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

**Unit IV: (18)**

**Bose-Einstein distribution:** Einstein condensation. Thermodynamic properties of ideal BE gas.
**Fermi-Dirac distribution:** Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

**Books Recommended:**

1. Statistical Mechanics, by Donald A McQuarrie
2. Introduction to Modern Statistical Mechanics, by David Chandler
3. Statistical Mechanics, by Kerson Haung
4. Statistical Mechanics, by Patria

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**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Physical Chemistry II**
**Paper Code: CHL.524**
**Total Lectures:** 54

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**Objective and Learning Outcomes:** The objective of this course is that students learn the advanced topics in physical chemistry, and gain depth knowledge in this fundamental branch of Chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in physical chemistry.

**Unit 1** **(14)**

**Electrochemistry:** Nernst equation, electrochemical cells, concentration cells with and without liquid junction, application of electrochemical cell, thermodynamics of reversible electrodes and reversible cells. activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law, conductometric titrations.

**Unit 2** **(14)**

**Reaction Kinetics:** Introduction, rates of chemical reactions, mechanisms of chemical reactions and steady state approximation, laws of photochemistry, kinetics of photochemical reactions, collision and transition state theories, stearic factor, treatment of unimolecular reactions, ionic reactions: salt effect.

**Unit 3** **(14)**

**Fast Reaction:** Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates, measurement of fluorescence and phosphorescence lifetimes, photoinduced electron transfer rates.

**Unit 4** **(12)**

**Adsorption and Catalysis:** Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Fredulich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Kinetics of catalytic reactions.

**Books Recommended:**


1. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5th Edition, 2011, MACMILLAN Publisher.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1stedition, 1998, Viva Books,.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4th Edition, 2004, Wiley-Interscience Publication.
7. Engel T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
8. Puri, B.R. Sharma L.R. and Pathania M.S. Principles of Physical Chemistry, 46th Edition, 2013, Vishal Publishing Company.
9. Laidler, K. J. Chemical Kinetics, 3rd Edition, 1987, Pearson Education Ltd.
10. Engel T. and Reid, P. Thermodynamics, Statistical Thermodynamics, & Kinetics, 3rd edition, 2013, Pearson Education.
11. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
12. Raj, G. Surface Chemistry (Adsorption), 4th Edition, 2002, Goel Publishing House.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Inorganic Chemistry II**
**Paper Code: CHL.521**
**Total Lectures:** 54

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**Objective and Learning Outcomes:** The objective of this course is that students learn the advanced topics in inorganic chemistry, and gain depth knowledge in this fundamental branch of Chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

**Unit 1** **(12)**

**Symmetry**

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination,

**Unit2** **(12)**

**Group theory**

Determination of reducible and irreducible representations, character tables, construction of character tables for C2v, C3v, use of symmetry in obtaining symmetry of orbitals in molecules.

**Unit3** **(14)**

**MetalComplexes**

Organic-transition metal chemistry, complexes with π-acceptor and σ-donor ligands, 18-electron and 16-electron rules, isolobal analogy, structure and bonding.Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygencomplexes, tertiary phosphine as ligand.metallocenes, metal cluster compounds, metal-metal bond, metal carbenes, carbonyl and non-carbonyl clusters, fluxional molecules, application of orgnaometallic compounds as catalysts in organic synthesis.

**Unit4** **(16)**

Inorganic chains, rings and cages

a) Chains: Catenation, heterocatenation, isopolyanions and heteropolyanions.

b) Rings: Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.

c) Cages: Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

**Books Recommended:**


1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2nd edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
7. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
8. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2nd edition, 1993, Affiliated East West Press.
9. Drago, Russell S. Physical Methods for Chemists, 2nd edition, 1992, Saunders College Publishing

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Organic Chemistry II**
**Paper Code: CHL.523**
**Total Lectures:** 54

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 0 | 0 | 3 | 75 |

**Objective and Learning Outcomes:** The objective of this course is that students learn the advanced topics in organic chemistry, and gain depth knowledge in this fundamental branch of Chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in organic chemistry.

**Unit 1** **(12)**

**Reactive intermediates:** Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.

**Aromaticity:** Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule, energy level of □-molecular orbitals, annulenes, azulenes, antiaromaticity.

**Unit 2** **(12)**

**Photochemistry:** Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

**Unit 3** **(16)**

**Pericyclic chemistry:**

Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5-hexatriene, Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.

**Electrocyclic reactions:** Conrotation and disrotation, 4n and 4n+2 systems. Woodward-Hoffmann rules. (i) Symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and correlation diagrams.

**Cycloaddition reactions:** Suprafacial and antarafacial interactions. π2 + π2 and π4 + π2 cycloadditions and stereochemical aspects. Diels-Alder reaction. Woodward-Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory

**Sigmatropic reactions:** [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [lj} shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

**Unit 4** **(14)**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

Selective Name Reactions: Sharpless asymmetric epoxidation, dihydroxylation, Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Stork-enamine, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin reaction.

**Books Recommended:**

1. Acheson, R.M. An introduction to the Chemistry of Heterocyclic Compounds, 3rd edition, 1976 Wiley India Pvt. Ltd.
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2nd edition, 2012, Oxford University Press.
3. Ahluwalia, V. K. and Parasar R. K. Organic Reaction Mechanism, 4th edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
4. Bansal, R. K. A Textbook of Organic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
5. Bansal R.K. Organic Reaction Mechanism,2010, New Age International (P) Ltd., New Delhi.
6. Bansal, R.K. Hetrocyclic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
7. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 4th edition, 2002, Kluwer Academic Publishers.
8. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 5th edition, 2007, Springer Science and Business Media Ltd.
9. Finar, I.L. Organic Chemistry Volume 1, 6th edition, 2012, Pearson Education UK.
10. Gilchrist, T.L. (1997). Heterocyclic Chemistry, 3rd edition, 1997, Addison Wesley Longman Publishers, US.
11. Gupta R.R., Kumar M. and Gupta V. Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3, 2010, Springer Verlag, India.
12. Joule, J.A. and Mills, K. Heterocyc1ic Chemistry, 5th edition,2010, Blackwell Publishers, New York.
13. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3rd edition, 2010, New Age International, New Delhi.
14. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3rd edition, 1998, Addison-Wesley Longman Inc., New York.
15. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6th edition, 2011, Prentice- Hall of India, New Delhi.
16. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3rd edition, 2009, Macmillan India Ltd., New Delhi.
17. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin V. V. Handbook of Heterocyclic Chemistry, 3rd edition, 2010, Elsevier UK.
18. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edition, 2013, John Wiley & Sons.
19. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6th edition, 1997, Prentice Hall.
20. Norman, R.O.C. and Coxon, J.M. Principles of Organic Synthesis, 3rd edition, 1998, Nelson Thornes, Blackie Academic & Professional.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Practical Physical Chemistry II**
**Paper Code: CHP.525**
**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

**Objective and Learning Outcomes:** The objective of this course is that student's get an in hand experience of experimental physical chemistry. This experience will help the students better appreciate how the experimental information gained in Chemistry can be enhanced with the help of Computational Modeling techniques that they will learn in subsequent semester of the programme.

1. Determination of strength of a given base by titrating with an acid conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.
3. Determination standard electrode potential of $Fe^{2+}/Fe^{3+}$ system by potentiometer using potassium permanganate solution.
4. Determination of $pK_a$ of acetic acid and glycine by pH meter using NaOH.
5. Determination of relative and absolute viscosity of a given liquid.
6. Determination of surface tension of alcohols.
7. Determination of refractive indices of given liquids.
8. Determination of concentrations of heme proteins using spectrophotometer
9. Preparation of buffers and measurement of their pH
10. Verification of the Lambert Beer's law.
11. Structural analysis of amino acids and proteins using FTIR and CD spectrometer.
12. Determination of the $T_m$ values of DNA and proteins.
13. Study of the thermal/cold denaturations of proteins using UV-visible and CD spectroscopic techniques.
14. Molecular weight of a non-electrolyte by cryoscopy method.
15. Determination of stability constant of Fe(III)-salicyclic acid complex by spectrophotometer.

**Books Recommended:**


Nad, A. K., Mahapatra, B. and Ghoshal, A. An Advanced Course in Practical Chemistry, 2014, New Central Book Agency (P) Ltd.
Maity S. and Ghosh, N. Physical Chemistry Practical, 2012, New Central Book Agency (P) Ltd.
Elias, A. J. Collection of Interesting General Chemistry Experiments, 2008, Universities Press.
Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, 2007, S. Chand& Sons.
Yadav, J.B. Advanced Practical Physical Chemistry, 2008, Krishna Prakasan Media.
Das, R.C. and Behra, B. Experimental Physical Chemistry, 1983, Tata McGraw-Hill.
James, A.M. and Prichard, F.E. Practical Physical Chemistry, 3rd edition, 1974, Longman, Harlow.
Ghosh, J.C., Experiments in Physical Chemistry, 1990, Bharati Bhavan.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Scientific Writing and IPR
**Paper Code: LBI.623**
**Total Lectures:** 54

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 2 | 2 | 0 | 3 | 75 |

**Unit I: Scientific Writing 1 (09)**

Introduction; principles of effective writing (cutting unnecessary clutter); Principles of effective writing (verbs); Crafting better sentences and paragraphs; Organization; and streamlining the writing process; The format of an original manuscript

**Unit II: Scientific Writing 2 (09)**

Reviews, commentaries, and opinion pieces; and the publication process; Issues in scientific writing (plagiarism, authorship, ghostwriting, reproducible research); How to do a peer review; and how to communicate with the lay public

**Unit III: International Conventions related to IPR (09)**

International convention relating to Intellectual Property - History of GATT & TRIPS Agreement – Berne convention-Madrid agreement-Hague agreement concerning the International Deposit of Industrial Designs –Patent Cooperation treaty (PCT)-Paris convention-Lisbon Agreement - Establishment of WIPO – UPOV and WTO-Mission and activities – History – General Agreement on Trade and Tariff (GATT)- TRIPS Trade-Related Aspects of Intellectual Property Rights – WCT and WPPT- Budapest Treaty - International Convention for the Protection of New Varieties of Plants –sui generis system

**Unit IV: IPR in Life Sciences and Computer related inventions (09)**

Patentability of Biotechnology Inventions - Protection of Genetic Resources - Patenting of seeds Moral Issues in Patenting Biotechnological Inventions – case studies on biotechnology patents -protection for Software and Computer related inventions - Protecting Trademark and Copyright in the Social media - Copyright Issues in the Digital Environment – case studies on computer related Inventions.

**Tutorials on:**

1. Patent search and Analytics

2. Patent strategy game shall be organized based on a real time situation for the students

**SEMESTER III**

**Objective and Expected Learning Outcomes:** The course structure of semester III of this Programme is designed

to provide students with courses that build their depth in the field of Computational Chemistry. This semester includes advanced courses in computational chemistry and foundation courses in computer programming. The list of courses to be taught in this semester is provided below.

**Course Title: Computational Methods**
**Paper Code: CSC.453**
**Total Hours: 72**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 3 | 2 | 0 | 4 | 100 |

**Unit I: (18)**

**Linear and Non –Linear equations:**
Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basic principles-Formulae-algorithms.

**Simultaneous equations:**
Solutions of simultaneous linear equations-Guass elimination and Gauss Seidel iterative methods-Basic principles-Formulae-Algorithms, Pivotal Condensation.

**Unit II: (18)**

**Matrix and Determinants:**
Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

**Unit III: (18)**

**Interpolations:**
Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms

**Numerical differentiation and integration:**
Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor's series, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration.

**Curve Fit:**
least square, straight line and polynomial fits.

**Unit IV: (18)**

**Numerical Solution of differential Equations:** Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

**Books Recommened:**

1. V. Rajaraman, Computer Oriented Numerical Methods, PHI.
2. Numerical Methods, E. Balaguruswamy, Tata McGraw Hill
3. F.Acton, Numerical Methods that Work, Harper and Row.
4. S. D. Conte and C.D.Boor, Elementary Numerical Analysis, McGraw Hill.
5. S. S. Shastri, "Introductory Methods of Numerical Analysis", PHI.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Computational Methods Lab**
**Paper Code: CSC.454**
**Total Hours: 36**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| - | - | 4 | 2 | 50 |

**Unit I: (18)**

**MATLAB:**
Basics of Mat lab- Mat lab windows – On-line help- Input-Output-File types-Platform Dependence-Creating and working with Arrays of Numbers – Creating, saving, plots printing Matrices and Vectors – Input – Indexing – matrix Manipulation-Creating Vectors Matrix and Array Operations Arithmetic operations-Relational operations – Logical Operations – Elementary math functions, Matrix functions – Character Strings Applications-

**Unit II: Application: (18)**

Jacobi Method of Matrix Diagonalization, Solution of transcendental or polynomial equations by the Newton Raphson method, Linear curve fitting and calculation of linear correlation coefficient, Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination, Finding Eigen values and eigenvectors, Matrix factorizations Curve Fitting – Polynomial curve fitting on the fly, Least squares curve fitting, General nonlinear fits, Lagrange interpolation based on given input data, Numerical integration using the Simpson's method, Numerical integrationg using the Gaussian quadrature method, Solution of first order differential equations using the Rung-Kutta method, Numerical first order differentiation of a given function, Fast Fourier Transform, Monte Carlo integration.

**Books Recommended:**


1. Y.Kirani Singh and B.B.Chaudhuri, MATLAB Programming, Prentice-Hall India, 2007
2. Rudra Pratap, Getting Started with Matlab 7, Oxford, Indian University Edition, 2006
3. Numerical Methods, E. Balaguruswamy, Tata McGraw Hill
4. Computer oriented numerical methods-Rajaraman


Semester II over

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Electronic Structure Theory**
**Paper Code: CSC.601**
**Total Hours: 72**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 1 | 0 | 4 | 100 |

**Objective and Learning Outcomes:** This is an advanced course for students who specialize in Computational Chemistry. The objective of this course is that students learn the techniques of molecular quantum chemistry and apply them to study chemical and biochemical problems.

**Unit I** **(18)**

**Many Electron atoms:** Electron correlation, addition of angular momentum, Clebesch-Gordan series, total angular momentum and spin-orbit interaction.

**Unit II** **(18)**

**Ab Initio Methods:** Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets.

**Unit III** **(18)**

**Electron Correlation and Basis Sets:** Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster, Basis sets.

**Unit IV** **(18)**

**DFT and Force Fields method:**Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

**Books Recommended:**


1. Introduction to Computational Chemistry, F. Jensen, 2nd edition, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 3rd edition, Oxford University Press, Oxford (1997).
3. Quantum Chemistry, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
4. Quantum Chemistry, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
5. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Electronic Structure Theory Lab**
**Paper Code: CSC.602**
**Total Hours: 36**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

**Course Objective and Learning Outcomes:** This course will provide practical experience to the students through use of important Computational Chemistry softwares.
Following experiments will be carried out in the lab.

1. Introduction to Gaussian calculations.
2. Carrying of conformational analysis of small molecules using G09.
3. Vibrational spectra, NMR spectra and TDDFT calculations using G09.
4. Modeling chemical reactions including transition state calculations.
5. 2D potential energy suface generation for two torsion angles.
6. Pseudopotential generation and testing of Si atom.
7. Functional and basis set dependent lattice constant and bulk modulus of Fe solid.
8. Total energy versus cell size and binding energy of $H_2$ and $H_2O$ molecules.
9. Density of states and electronic band structure of bulk Si.
10. To study the structural and electronic properties of graphene and its nanoribbon.
11. Building macromolecules, extracting crystal structure/NMR coordinates and generating models for MD simulations. RESP charge calculation.
12. Energy minimization during MD simulations- Steepest descent and conjugate gradient methods.
13. Gas phase MD simulations.
14. MD simulations in implicit solvent.
15. MD simulations in Explicit solvents.

**References:**

1. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
2. http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.html
3.http://blogs.cimav.edu.mx/daniel.glossman/data/files/Libros/Exploring%20Chemistry%20With%20Electronic%20Structure%20Methods.pdf
4. http://ambermd.org/tutorials/

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Fundamentals of Molecular Simulations**
**Paper Code: CSC.603**
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Course Objective and Learning outcomes:** The objective of this subject is to ensure that a student learns modelling of molecular structures and understanding the dynamics of the structural transitions, which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

**Unit I (18)**

**Molecular Modeling and Structure** - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.
**Force Fields and Molecular Representation** – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints, (e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?
Example: Protein, Nuclic Acid, Small Molecule Force Field, Water Models.

**Unit II (18)**

**Methods for Simulating Large Systems**
(a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists, (b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary, (c) Long-range Interactions – The Ewald Sum, The Reaction Field Method

**Unit III (18)**

**Energy Minimization and Related Analysis Techniques**
(a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum?
Introduction to Equilibrium Statistical Mechanics
(a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles (c) Statistical Mechanics of Fluids

**Unit IV (18)**

**Simulation Methods:**
**Monte Carlo:** (a) MC integration and Markov chains, (b) The Metropolis method, (c) Biased MC
**Molecular Dynamics:** (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method, Nose-Hoover Dynamics, (f) Pressure Control: Andersen's Method, Nose-Hoover Method, Rahman-Perrinilo Method, (g) Calculating properties from MD trajectories, (h) Hybrid MC,
**Free Energy:** (a) Perturbation Methods, (b) TI (Thermodynamic Integration)
Brownian dynamics and the Langevin Equation.

**Books Recommended:**

1. Computer Simulation of Liquids, by M.P. Allen and D.J. Tildesley, (QC 145.2.A43 1992)
2. Understanding molecular simulation, by Daan Frenkel and Berend Smit, (QD 461 .F86 1996)
3. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Molecular Simulations Lab**
**Paper Code:** CSC.604
**Total Lecture:** 36

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

**Course Objective and Learning outcomes:** The objective of this subject is to ensure that a student gains practical in-hand experience of various modeling and classical simulation tools, including, but not limited those that are used in macromolecular modeling. The course will help the students learn the use the techniques of molecular simulations, which will enhance their employability in their further potential carrers in academia and industry.

Advanced Visualization Software and 3D representations with VMD and Rasmol.
Coordinate generations and inter-conversions.
Secondary Structure Prediction.
Fold Recognition, *ab initio method.*
Homology based comparative protein modeling.
Energy minimizations and optimization.
Validation of models.
- a WHATIF
- b PROSA
- c PROCHECK
- d VERIFY 3D

Protein Structure Alignment.
Modeller
Structure based Drug Design
- a Molecular Docking
- b De Novo Ligand Design
- c Virtual Screening

Ligand based Drug Design
- a Pharmacophore Identification
- b QSAR

12. Molecular Dynamics with Gromacs
13. Binding Site Identification

**Books Recommended:**

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Seminar in Computational Science**
**Paper Code: CSC.499**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:

| S.No. | Criteria | Marks |
|---|---|---|
| 1 | Content | 20 |
| 2 | Presentation Skills | 20 |
| 3 | Handling of queries | 10 |

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Molecular Spectroscopy
**Paper Code:** CSC.605
**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Objective and Learning Outcomes:** This is a fundamental course for students who specialize in Physical/Computational Chemistry. The objective of this course is that students learn the basic concepts of molecular spectroscopy from a fundamental point of view. The course will help students to understand how spectroscopic transitions come into picture in molecular quantum mechanics.

**Unit I** **(20)**

**Basic Principles:** Interaction of electromagnetic radiation with matter, time-dependent perturbation theory, harmonic perturbation and transition probabilities, Einstein transition probabilities, selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy. Introduction to Electronic spectra, Born-Oppenheimer approximation, Franck–Condon principle, change of shape on excitation, Jablonski diagram: fluorescence and phosphorescence.

**Unit II** **(20)**

**Infra-red and Raman Spectra:** Harmonic and anharmonic oscillators, fundamental frequencies, overtones, Morse potential, hot bands, vibration-rotational spectra of HCl, P, Q, R branches, vibrational theories of polyatomic molecules, normal coordinates and their symmetry ($CO_2$). Molecular polarizability–Raman Effect, pure rotational Raman spectra of linear molecules, vibrational Raman spectra–Raman activity of vibrational, rule of mutual exclusion. Microwave spectra: rigid and non-rigid rotator mode ls, rotational energies of diatomic molecules: moment of inertia and bond length, centrifugal distortion, effect of isotopic substitution.

**Unit III** **(14)**

**Magnetic Resonance:** Basic Principles, Nuclear Shielding, Chemical Shift, Spin-spin Coupling: AX, AMX, $AX_2$, $AX_3$, $AX_n$, Equivalent Nuclei, Mechanism, Dipolar Coupling.

**Unit IV** **(18)**

**Lasers and Laser Spectroscopy:** Principles of laser action, laser characteristics, pulsed lasers, laser cavity modes, Q-switching, mode locking, non-linear effects, harmonic generation, examples of lasers: He-Ne, Nd-YAG, dye lasers, femtosecond spectroscopy.

**Books Recommended:**


1. Modern Spectroscopy, J. M. Hollas, 4th edition, John Wiley & Sons, Ltd. (2004).
2. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill (1962).
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, Tata McGraw Hill, New Delhi (1994).
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3rd Edition, Springer.
5. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, Chapman and Hall, London (1979).
6. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, Addison Wesley, Longman Ltd, London (1986).

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Introduction to Biochemistry

**Paper Code:** CSC.606

**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Objective**: This objective of the subject is to ensure that a student understands the structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles, and how chemical forces and reactions determine their structure and functions in living cells.

**Unit I** **(18)**

**Composition, structure and function of Biomolecules:** Carbohydrates, Lipids, Proteins, Nucleic acids and Vitamins. Bioenergetics and metabolism of Carbohydrates, Lipids, Amino Acids and Nucleotides.Stabilizing interactions in biomolecules: Van der Waals, Electrostatic, Hydrogen bonding,Hydrophobic interactions, etc.

**Unit II** **(18)**

**Protein and Nucleic Acid Chemistry:**The three dimensional Structure of Proteins Ramachandran plot, Secondary, Tertiary and Quaternary structure, Domains, Motif and Folds. Nucleic acids: A-, B-, Z-DNA, 3D RNA structures, folding and recognition, Stability of protein and Nucleic acid structures.

**Unit III** **(18)**

**Replication, transcription and translation processes:** Proposed Mechanisms of reactions and enzymes involved.
**Enzymology:** Classification, Principles of catalysis, Mechanism of enzyme catalysis, Enzyme kinetics, Enzyme regulation, Isozymes Clinically important enzymes.

**Unit IV** **(18)**

**Biosynthesis:** Biosynthesis of Amino Acids, Nucleotides, and Related Molecules, DNA, RNA and Protein metabolism, Regulation of gene expression.

**Books Recommended:**


1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry.* W.H. Freeman & Company. USA.
2. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction*. Blackwell Publishing Professional. USA.
3. Haynie, D.T. (2007). *Biological thermodynamics*. Cambridge University. UK.
4. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). *Biochemistry*.Oxford University Press Inc. New York.
5. Nelson, D. and Cox, M.M. (2008). *Lehninger Principles of Biochemistry*.BI publications Pvt. Ltd. Chennai, India.
6. Ochiai, E. (2008). *Bioinorganic chemistry: A survey.* Academic Press. Elsevier, India.
7. Randall, D. J., Burggren, W. and French, K. (2001). *Eckert animal physiology*. W.H. Freeman & Company. USA.
8. Raven, P.H., Johnson, G.B. and Mason, K.A. (2007). *Biology*. Mcgraw-Hill. USA.
9. Shukla AN (2009). *Elements of enzymology.* Discovery Publishing. New Delhi, India.
10. Voet, D. and Voet, J.G. (2008). *Principles of biochemistry*. CBS Publishers & Distributors. New Delhi, India.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Density Functional Theory
**Paper Code:** CSC.607
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Objective and Learning Outcomes**: This is a specialization course for students of Computational Chemistry. The objective of this course is to make the students understand the basics of Density Functional Theory (DFT), which is a popular electronic structure method. With the increasing power of computers, DFT-based calculations are emerging as a useful tool to characterize the properties of molecules and materials. This course will review the various theories/approximations necessary to understand most popular framework of modern DFT.

**Unit-I** **(18)**

**Many-body Approximations:** Schrodinger equation and its solution for one electron and two electron systems, Hamiltonian of many particles system, Born-Oppenheimer approximation, Hartree theory, Idea of self consistency, Exchange energy and interpretation, Identical particles and spin, Hartree-Fock theory, Antisymmetric wavefunctions and Slater determinant, Koopmans' theorem, Failures of Hartree-Fock in solid state, Correlation energy, Variational principle, Connection between Quantum Mechanics,Variational Principle and Classical Mechanics.

**Unit-II** **(18)**

**From Wave Functions to Density Functional:** Idea of functional, Functional derivatives, Electron density, Thomos Fermi model, Hohenberg-Kohn theorems, Approximations for exchange-correlation: Local density approximation (LDA) and local spin density approximation (LSDA), Gradient expansion and generalized gradient approximation (GGA), Hybrid functionals and meta-GGA approaches. Self-interaction corrections (SIC).

**Unit-III** **(18)**

**Practical Implementation of Density Functional Theory (DFT):** Kohn-Sham formulation: Plane waves and pseudopotentials, Janak's theorem, Ionization potential theorem, Self consistent field (SCF) methods, Understanding why LDA works, Consequence of discontinuous change in chemical potential for exchange-correlation, Strengths and weaknesses of DFT.

**Unit-IV** **(18)**

**Electronic Structure with DFT:** Free electron theory, Band theory of solids, Tight-binding method, Semiconductors, Band structure, Density of states. Interpretation of Kohn-Sham eigenvalues in relation with ionization potential, Fermi surface and band gap.

**Books Recommended:**


1. Richard M. Martin, Electronic Structure: Basic Theory and Practical Methods, (Cambridge University Press, 2004)
2. Robert G. Parr and Weitao Yang, *Density Functional Theory of Atoms and Molecules*, (Oxford University Press, 1994).
3. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
4. June Gunn Lee, *Computational Materials Science: An Introduction*, (CRC Press 2011)
5. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Introduction to Quantum Dynamics
**Paper Code:** CSC.608
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 1 | 0 | 4 | 100 |

**Course Objective and Learning Outcomes:** This course will introduce the basic aspects of time dependent quantum wavepacket dynamics to Masters students.

**Unit I**[1-6] **18 Hours**

**Separation of electronic and nuclear motions:** adiabatic representation, Born-Oppenheimer approximation, Hellmann-Feynman theory, diabatic representation, transformation between two representations, crossing of adiabatic potentials.

**TDSE:** separation of variables and reconstitution of the wavepacket, expectation values, free-particle wavepacket: centre and dispersion of the wavepacket.

**Unit II**[1-6] **18 Hours**

Gaussian wavepacket: Gaussian free particle, general properties of Gaussian wavepackets, Gaussian in a quadratic potential. Correspondence between Classical and Quantum Dynamics: Ehrenfest's Theorem, Bohmian Mechanics and the Classical limit.

**Unit III**[1-4] **18 Hours**

Spectra as Fourier transforms of wavepacket correlation functions. 1D barrier scattering: wavepacket formulation of reflection and transmission coefficients, cross-correlation function and S-matrix.

**Unit IV**[1-6] **18 Hours**

Numerical methods for solving the TDSE: spectral projection and collocation, pseudospectral basis, gaussian quadrature, represntation of the hamiltonian in the reduced space, discrete variable representation, Fourier method, time propagation.

**Books**

1. D. J. Tannor, *Introduction to Quantum Mechanics: A Time-dependent Perspective*, University Science Books, 2006.
2. Edited by R E Wyatt and J Z H Zhang, *Dynamics of Molecules and Chemical Reactions*, CRC Press, 1996.
3. K. C. Kulander, *Time-dependent Methods for Quantum Dynamics*, Elsevier Science, 1991.
4. J. Z. H. Zhang, *Theory and application of Quantum Molecualr Dynamics*, World Scientific Publishing Company, 1998.
5. Edited by M Brouard and C Vallance, *Tutorials in Molecular Reaction Dynamics*, Royal Society of Chemistry, 2010.
6. Edited by D. A. Micha, I. Burghardt, *Quantum Dynamics of Complex Molecular Systems*, Springer-Verlag, 2006.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title:** Statistics for Chemical and Biochemical Applications
**Paper Code:** CSC.609
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Unit I** **(15)**

**Overview of Biostatistics:** Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

**Unit II** **(15)**

**Descriptive statistics:** Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

**Unit III** **(18)**

**Experimental design and analysis:** Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

**Unit IV** **(24)**

**Inferential Statistics:** Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, $\chi^2$ test. Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

**Books Recommended:**


1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley, USA.
2. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc. USA.
3. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials.* 3/e (with SPSS). Decker Inc. USA.
4. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*. W.H. Freeman publishers, USA.
5. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley, USA.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: M.Sc. Project work**
**Paper Code:** CSC.611

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 32 | 16 | 400 |

**Objective and Learning Outcome:** The objective of this course would be to ensure that the student carries research in the topic chosen. The evaluation criteria for this course shall be as follows:

Maximum Marks: 400

| S.No. | Criteria | Marks |
|---|---|---|
| 1. | Continuous assessment by the supervisor | 100 |
| 2. | First mid-semester presentation (synopsis) | 100 |
| 3. | Second mid-semester presentation (presubmission) | 100 |
| 4. | Final presentation and Defense | 100 |
| Total | | 400 |

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Biomolecular Modeling and Drug Designing Lab**
**Paper Code: CSC.612**
**Total Lectures:** 36

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 0 | 0 | 4 | 2 | 50 |

**Course Objective and Learning Outcomes:** The objective of this subject is to ensure that a student learns practical aspects of modelling of biomolecular structures.

The following experiments should be conducted by the students:
A. Molecular Recognition
1. Prediction of Protein-ligand interaction sites
2. Prediction of Protein-protein interaction sites
3. Prediction of Protein-membrane interaction sites
4. Prediction of Protein-nucleic acid interaction sites

B. Docking
1. Protein Ligand Docking using
(i) Autodock
(ii) Vina
(iii) Dock
2. Protein-protein docking by HADDOCK or other similar methods

C. Modelling macromolecular structure
1. Homology modeling
2. *ab-initio* structure modeling

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Biomolecular Modeling and Drug Designing**
**Paper Code: CSC.613**
**Total Lectures:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 1 | 0 | 4 | 100 |

**Unit I: (18)**

**Introduction:** What is Biomolecular Modeling and the importance of Biomolecular Simulation. Principles of protein and nuclic acid structure: Tertiary structure, Qaternary structure, Similarity of ternary and quaternary structure

**Protein secondary structure:** Introduction, Hydrogen bond, Defining a secondary structure element, Methods for predicting secondary structure

**Experimental methods for protein structure determination**: X-ray crystallography, Nuclear magnetic resonance (NMR)

**Unit II: (18)**

**Basic concepts:** Units and derivatives, Force field and energy landscape, Truncation of nonbonded interactions

**Conformational Sampling:** Minimization and alogrithms, Molecular dynamics, Ensembles (statistical mechanics), Monte Carlo simulations

**Solvation:** Periodic boundary condition, Ewald summation, Implicit solvent model and continuum electrostatics, Monte Carlo simulation on parallel computers

**Advanced Techniques:** Replica-exchange molecular dynamics, Restraint potentials, Free energy calculations, Membrane simulations

**Unit III: (18)**

**Protein tertiary structure modeling:** Basic concepts, Protein folding and dynamic simulation, Modeling protein sidechains, Comparative modeling, Threading, Ab initio modeling, Combined modeling approaches, CASP: A blind protein structure prediction competition

**Introduction to protein design:** "Rational" design efforts, Experimental methods (directed evolution), Computational protein design

**Unit IV: (18)**

**Protein Interaction**

**Protein quaternary structure modeling:** Basic concepts, Energy landscapes, Docking algorithms – foundation, Docking algorithms – current & future, Docking example, CAPRI, Protein Structure Initiative, Computational proteomics

**Designing protein-protein interfaces:** Designing for affinity, Designing for specificity

**Books Recommended:**


1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Advanced Statistical Mechanics and Molecular Reaction Dynamics**
**Paper Code: CSC.614**
**Total Lecture: 72**

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 1 | 0 | 4 | 100 |

**Unit I** **(18)**

Review of Statistical Mechanical concepts, Phases & Phase Transitions: The Ising Model : Stability of Thermodynamics Phases, First-order Phase transitions, Interfaces, The Ising Model, Lattice Gas, Broken Symmetry, Mean Field Theory.

**A brief introduction to Liquid Theory:** Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids

**Atomic and continuum models of liquids:** The Lennard-Jones Fluid, Molecular dynamics simulation, Correlation functions and measurements, elements of linear response theory, Linear models (a) Langevin equations (diffusion, friction and memory). (b) Gaussian fields (Debye-Huckel and beyond), The hard sphere model, WCA theory, Chemical equilibrium and relaxation.

**Unit II** **(18)**

**Non-equilibrium systems:** Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis
Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions.

**Special topics:** Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Path integrals, Tunneling—instantons, Ising model / Quantum correspondence, Monte Carlo and Biased Monte Carlo methods.

**Unit III** **(18)**

**Potential Energy Surfaces:** Long-range Potentials, Empirical Intermolecular Potentials, Molecular Bonding Potentials, Internal Coordinates and Normal Modes of Vibration, Ab Initio Calculation of Potential Energy Surfaces, Analytic Potential Energy Functions, Details of the Reaction Path.Dynamics of Bimolecular Collisions: Simple Collision Models, Two-Body Classical Scattering, Complex Scattering Process.

**Unit IV** **(18)**

**Transition State Theory:** Basic Postulates and Derivation of Transition State Theory, Dynamical Derivation of Transition State Theory, Quantum Mechanical Effects in Transition State Theory, Thermodynamic Formulation of Transition State Theory, Applications of Transition State Theory.Unimolecular Reaction Dynamics: The Lindmann-Hinshelwood Mechanism, Statistical Energy-dependent Rate Constant, RRKM Theory, Applications of RRKM Theory to Thermal Activation.

**Books Recommended:**


1. Statistical Mechanics, by Kerson Haung
2. Statistical mechanics, by Patria
3. B. K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi (1998).
4. D. A. Mcquarrie, Statistical Mechanics, University Science Books (2011).
5. D. Chandler, Introduction to Statistical Mechanics, Oxford University Press (1987).
6. B. Widom, Statistical Mechanics- A concise Introduction for Chemists, Cambridge University Press (2002).
7. Terrell L. Hill, Statistical mechanics: principles and selected applications, Courier DoverPublications (1987).
8. J. I. Steinfeld, J. S. Francisco, and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall (1998).
9. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press (2009).
10. N. E. Henriksen F. Y. Hansen, Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics, Oxford University Press, USA (2012).
11. M. Brouard, Reaction Dynamics, Oxford Chemistry Primers (1998).
12. P. L. Houston, Chemical Kinetics and Reaction Dynamics, Dover Publications (2012).
13. S. K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer (2006).
14. K. J. Laidler, Chemical Kinetics, Pearson (2008).
15. A. H. Zewail, Femtochemistry-Ultrafast Dynamics of the Chemical Bond, World Scientific, New Jersey (1994).

**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

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**Course Title: Modeling Polymeric Materials**
**Paper Code:** CSC.615
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 0 | 0 | 4 | 100 |

**Course Objective and Learning Outcomes:** This course will introduce the modelling of materials through modern computational tools to analyze materials at nanoscale. It is an initiative to make students familiar with the power of first principles electronic structure theory techniques.

**Unit-I** **(18)**

**Materials Modelling through VASP and SIESTA:** Basis Sets: plane waves versus numerical atomic orbitals basis sets, Pseudopotentials: ultrasoft versus norm conserving pseudopotentials. Numerical solutions of Kohn-Sham equations, Diagnolization procedure, SCF cycles and mixing scheme, Smearing: Gaussian, Fermi and Methfessel-Paxton smearing.
SIESTA and VASP package to perform: electronic structure calculations, relaxation of atomic positions and unit cell parameters. Structural properties: equilibrium lattice constant, cohesive energy, bulk modulus.

**Unit-II** **(18)**

**DFT Calculations for Simple Solids:** Crystal structure, Reciprocal lattice, Bonding in crystal, Supercells, Face centered cubic materials, Hexagonal closed packed materials, Crystal structure prediction, Phase transformations, Reciprocal space and k-points**,** Choosing k-points in Brillouin zone, Energy Cutoff, DFT total energies and its relation to various properties, Geometry optimization. Electronic density of states, local density of states and atomic charges, Magnetism.

**Unit-III** **(18)**

**DFT Calculations for Surfaces:** Periodic boundary conditions and slab model, Calculations of surface energies, Symmetric and asymmetric slab model, Surface relaxation, Surface reconstruction, Adsorbate on surface, Surface Coverage, modelling of one-dimensional systems such as nanotubes, nanoribbons and nanowires, modelling of fullerene-like cages.
**DFT Calculations of Vibrational Frequencies:** Lattice vibrations and phonons,Isolated Molecules, Vibrations of a collection of atoms, Molecules on surface, Zero-point energies, Phonons and delocalization modes.

**Unit-IV** **(18)**

**Calculations beyond Standard DFT:** Accuracy of DFT calculations: energy, geometry, vibrational frequencies, Crystal structures and cohesive energies, adsorption energies and bond lengths. DFT+U and DFT+D method for the treatment of electron correlation, Spin-orbit coupling, GW approximation, Excited states properties: dielectric functions and absorption spectra.

**Books Recommended:**


1. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
2. June Gunn Lee, *Computational Materials Science: An Introduction*, (CRC Press 2011)
3. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007
4. www.vasp.at/index.php/documentation
5. http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.htm


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**CENTRE FOR COMPUTATIONAL SCIENCES**
**CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001**

**Course Title: Physical Organic Chemistry**
**Paper Code:** CSC.616
**Total Lecture:** 72

| L | T | P | Credits | Marks |
|---|---|---|---|---|
| 4 | 1 | 0 | 4 | 100 |

**Total Lecture:** 72

This course on Physical Organic Chemistry will provide conceptual understanding of chemical bonding, aromaticity, structure and stereochemistry, steric and conformational properties, chemical reactivity, correlation of structure with reactivity, Hammond postulates, solvent effects, acidity, nucleophilicity, electrophilicity, studying reaction mechanisms, isotope effects Woodward Hoffmann rules.

**Unit-I**[1-6] **(18)**

Chemical bonding: Covalency and molecular structure, approximate molecular orbital theory, properties of covalent bonds, intermolecular forces, aromaticity, structure. Woodward Hoffmann rules.

Unit-II[1-6] **(18)**

Correlation of structure with reactivity: Electronic demands, the Hammett equation, substituent constants σ, theories of substituent effects, interpretation of σ-values, reaction constants, ρ, deviations from the Hammett equation, dual-parameter correlations, molecular orbital considerations, cross-interaction terms

Unit-III[1-6] **(18)**

Steric and conformational properties: Origins of steric strain, examples of steric effects upon reactions, measurement of steric effects upon rates.

Solvent effects: structure of liquids, solutions, solvation, thermodynamic measures of solvation, effects of solvation on reaction rates and equilibria, empirical indexes of solvation, use of solvation scales in mechanistic studies.

Unit-IV[1-6] **(18)**

Kinetic isotope effects: isotopic substitution, theory of isotopic effects, transition-state geometry, secondary kinetic isotope effects, heavy atom isotope effects, tunnel effect

Acids and bases, nucleophiles and electrophiles: acid-base dissociation, the strengths of oxygen and nitrogen acids, linear free-energy relationships, rates of proton transfers, structural effects on amine protonation, factors that influence carbon acidity, theories of proton transfer, nucleophilicity and electrophilicity and their measurement.

**Recommended Readings:**


1. Neil S. Isaacs, *Physical Organic Chemistry*, 2nd Edition, PHI, 1995.
2. E. V. Anslyn & D. A. Dougherty, *Modern Physical Organic Chemistry*, Illustrated Edition,University Science Books, 2005.
3. Francis A. Carey and Richard J. Sundberg, *Advanced Organic Chemistry*, Part A, Structure and Mechanisms, 5th edition, Springer, 2007.
4. Jerry March, *Advanced Organic Chemistry, Reactions, Mechanims and Structure*, 4th Edition, John-Wiley, 1999.
5. Thomas H. Lowry, Kathleen S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd Edition, Harper & Row, 1981.
6. S. P. Gupta, *QSAR and Molecular Modeling*, Anamaya Publishers, 2011.